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Thermal emission spectrum of the new intermetallic molecule : CoCu

K N Uttam and M M Joshi
Saha's Spectroscopy Laboratory, Department of Physics, Allahabad University, Allahabad-211 002, India

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Abstract : The emission spectrum of the mixed vapours of cobalt and copper has been investigated for the first time at 2400°C in an atmosphere of argon. About 51 bands, degraded to violet, have been recorded and are attributed to four systems viz. A, B, C and D. The vibrational analyses have been carried out and the carrier of the bands has been identified as the diatomic CoCu. Vibrational constants have been determined for the different systems

Keywords : Thermal emission, molecular spectra, vibrational analysis

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Electronic spectra of the thermal plasma of metals or alloys have led to the identification of several gaseous intermetallic diatoms. Though transition elements occupy significant positions in the periodic table due to involving partially filled '*d*' orbital in their electronic structures, their diatomic molecules involving transition elements are not much known. Since NiCu molecule has been reported recently [1], we expect a formation of CoCu, FeCu molecules. It was with a view to studying the spectra of such molecules that this investigation was under taken.

The present report presents an account of the authors' findings on new intermetallic diatomic emitter *viz.* CoCu. The band spectra attributed to CoCu molecule has been obtained in thermal plasma using high temperature vacuum graphite furnace.

A small quantity of the intimate mixture of cobalt and copper (Johnson Matthey) was put into the experimental tube of Saha's high temperature graphite furnace. After evacuation of the furnace chamber, argon gas was filled at about a pressure of 50 cm of Hg to avoid rapid effusion of the molecular vapours from the open ends of the graphite tube. The graphite tube was electrically heated to about 2400°C. The spectra were photographed on 400 ASA

ORWO black and white film using two meter Plane Grating Spectrograph (PGS-2) with a grating blazed at λ 5600 Å and total lines ruled 45600. Exposures of the order of 13 to 15 minutes were sufficient to obtain a satisfactory impression of the emission spectrum at a reciprocal linear dispersion of 7.3 Å/mm in first order of PGS-2. An iron d.c. arc spectra were used for comparison. The measurements were performed using C.Z. Abbe Comparator.

Thermal emission spectrum, attributed to CoCu, has been recorded for the first time in the spectral region $\lambda\lambda$ 6100–6400 Å. About 51 bands have been photographed and analyzed into four systems *viz.* A, B, C and D. All the bands are single headed and degraded to lower wavelength side. Out of the 51 bands, the system A–X consists of 11 while systems B–X, C–X and D–X comprise 15, 14, 11 bands respectively. The observed bands have been satisfactorily analyzed yielding the following constants :

System	ν_{00}	ω_e'	$\omega_e'x_e'$	ω_e''	$\omega_e''x_e''$
A	16092.6	275.0	0.5	273.0	1.4
B	16122.2	274.0	0.6	273.0	1.4
C	16201.0	276.0	0.8	273.0	1.4
D	16246.4	274.0	0.5	273.0	1.4

The band head data together with the visual estimates of intensities and their classifications are collected in Table 1. The spectrogram could not be reproduced because of the poor contrast. Bands of these systems are, however, discernible under the comparator and can be measured.

The following facts support the assignment of the present spectrum to the diatomic CoCu molecule.

The new bands appear only when the experimental mixture (cobalt and copper metal) was put into the graphite tube and no band appeared when the clean and empty tube was heated to the same degree and the spectrum of the emergent light was photographed. This fact indicates that the spectrum is not due to any impurity in the graphite tube. Further, cobalt and copper of different makes were put inside the tube and heated under the same operational conditions. In each of these cases, the same group of bands as reported here, appeared invariably. It can therefore, be safely concluded that the present spectrum is due to CoCu molecule.

Vibrational analysis of the spectrum due to CoCu establishes the ground state vibrational frequency to be about 270.0 cm^{-1}. This value lies between the ω_e'' values of Co_2 (280.0 cm^{-1}) and Cu_2 (266.1 cm^{-1}). This is also in accordance with the value expected from empirical considerations of ground state frequencies of the molecules Co_2 [2] and Cu_2 [3]. The bands appear in the region $\lambda\lambda$ 6100–6400 Å, where no bands due to the molecule Co_2 and Cu_2 are known to be present in thermal emission. Low dispersion of the spectrograph

used, did not permit to make a study of the isotopic effect. In view of the above facts, it appears that the assignments are quite convincing.

Table 1. Band head data of CoCu molecule.

ν_{cal} (cm^{-1})	ν_{obs} (cm^{-1})	Int.	analysis (v', v'')	ν_{cal} (cm^{-1})	ν_{obs} (cm^{-1})	Int.	analysis (v', v'')
	A – X system				B – X system		
15822.4	15821.5	1	(0, 1)	15852.0	15853.2	1	(0, 1)
15829.0	15829.5	1	(1, 2)	15857.4	15856.3	1	(1, 2)
15837.4	15837.3	1	(2, 3)	15864.4	15864.3	1	(2, 3)
15847.6	15846.0	1	(3, 4)	15873.0	15874.5	1	(3, 4)
15859.6	15859.8	1	(4, 5)	15883.2	15881 8	1	(4, 5)
15873.4	15872.6	1	(5, 6)	15895.0	15894.9	1	(5, 6)
15889.0	15891.0	1	(6, 7)	15908.4	15907.2	1	(6, 7)
16092.6	16092.6	5	(0, 0)	15923.4	15924.2	1	(7, 8)
16096.4	16095.8	4	(1, 1)	16122.2	16122.2	4	(0, 0)
16102.0	16101.9	1	(2, 2)	16124.8	16125.3	3	(1, 1)
16109.4	16107.9	1	(3, 3)	16129.0	16129.5	4	(2, 2)
	C – X system			16134.8	16135.3	4	(3, 3)
15930.8	15931.4	1	(0, 1)	16142.2	16140.8	3	(4, 4)
15937.8	15936.5	1	(1, 2)	16151.2	16152.0	3	(5, 5)
15946.0	15945.6	1	(2, 3)	16161.8	16162 3	3	(6, 6)
15955.4	15955.7	1	(3, 4)		D – X system		
15966.0	15967.3	1	(4, 5)	15976.2	15976.4	1	(0, 1)
15977.8	15976.4	1	(5, 6)	15981.8	15982.2	1	(1, 2)
15990.8	15990.3	1	(6, 7)	15989.2	15988.0	1	(2, 3)
16005.0	16004.9	1	(7, 8)	15998.4	15997.3	1	(3, 4)
16201.0	16201.0	3	(0, 0)	16009.4	16008.3	1	(4, 5)
16205.2	16205.1	2	(1, 1)	16246.4	16246.4	2	(0, 0)
16210.6	16210.9	2	(2, 2)	16249.2	16250.1	2	(1, 1)
16217.2	16216.1	1	(3, 3)	16253.8	16253.9	1	(2, 2)
16225.0	16224.9	1	(4, 4)	16260.2	16261.2	1	(3, 3)
16234.0	16233.0	1	(5, 5)	16268.4	16270.0	1	(4, 4)
				16278.4	16275.4	1	(5, 5)

The dissociation energy of CoCu molecule, using Birge-Sponer formula is given by

$$D_0 = \omega_e''^2 / 4\omega_e'' x_e''$$

Substituting the values, we find $D_0 = 13308.7\ cm^{-1} = 1.65$ eV. This value is very near to the reported value 1.62 eV.

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